On the role of electron correlation and disorder on persistent currents in isolated one-dimensional rings

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Abstract

To understand the role of electron correlation and disorder on persistent currents in isolated 1D rings threaded by magnetic flux ϕ , we study the behavior of persistent currents in aperiodic and ordered binary alloy rings. These systems may be regarded as disordered systems with well-defined long-range order so that we do not have to perform any configuration averaging of the physical quantities. We see that in the absence of interaction, disorder suppresses persistent currents by orders of magnitude and also removes its discontinuity as a function of ϕ . As we introduce electron correlation, we get enhancement of the currents in certain disordered rings. Quite interestingly we observe that in some cases, electron correlation produces kink-like structures in the persistent current as a function of ϕ . This may be considered as anomalous Aharonov-Bohm oscillations of the persistent current and recent experimental observations support such oscillations. We find that the persistent current converges with the size of the rings.

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1 Introduction

In the mesoscopic and nanoscopic world phase coherence of the electronic states are of fundamental importance, and the phenomenon of persistent current is a spectacular consequence of quantum phase coherence in these regimes. In a pioneering work Büttiker, Imry, and Landauer [1] suggested that even in the presence of impurity, a small conducting isolated ring enclosing a magnetic flux ϕ carries a current in the ground state, a current which persists (does not decay) in time, and periodic in ϕ with periodicity $\phi_0 = ch/e$, the elementary flux quantum. Since then the phenomenon of persistent current in mesoscopic systems has been discussed quite extensively in the literature both theoretically [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15] as well as experimentally [16, 17, 18, 19, 20]. However, till now the observed experimental features of the persistent currents are not well-understood theoretically. A typical example of such discrepancy between theory and experiment is that the amplitude of the measured persistent currents are orders of magnitude larger than the theoretical predictions. It is believed that the electron-electron correlation and disorder have major role on the enhancement of persistent currents, but no consensus has yet been reached. Another controversial issue is that experimentally both ϕ_0 and $\phi_0/2$ periodicity has been observed, and it is also found that the $\phi_0/2$ oscillations near zero magnetic field exhibit diamagnetic response. The explanation of these results in terms of the ensemble averaged persistent currents is also quite intriguing, and the calculations show that the disorder averaged current crucially depends on the choice of the ensemble [4, 5]. In order to reveal the role of disorder and electron correlation on the persistent currents, in this work we focus attention on certain systems which closely resemble the disorder systems where we do not require any configuration averaging. These are chemically modulated structures possessing well-defined long-range order, and, as specific examples we consider the aperiodic and ordered binary alloy rings. We confine ourselves to small 1D rings where persistent currents can be calculated exactly, and we obtain many interesting new

results as a consequence of electron correlation and disorder. One such result is the enhancement of persistent currents in these systems due to electron correlation. Another important observation is the appearance of kink-like structures in the persistent current due to electron-electron correlation, which may be considered as anomalous Aharonov-Bohm oscillations. With the recent advancements in sub-micron technology, such systems can be easily fabricated in the laboratory, and in fact, in a recent experiment Keyser et al. [20] reported similar anomalous Aharonov-Bohm oscillations from the transport measurements on small rings with less than ten electrons. Our study may also be helpful to understand the physical properties of Benzene-like rings, and other aromatic compounds in the presence of magnetic flux.

This paper is organized as follows. In section 2, we present the calculation of persistent currents in ordered binary alloy rings and investigate their behavior in the presence of Coulomb repulsion. In section 3, we describe our results for the incommensurate rings in the presence of electron-electron interaction. Lastly, we conclude in section 4.

2 Ordered binary alloy rings

In this section we describe the current-flux characteristics for the ordered binary alloy rings at T=0. We use the tight-binding Hubbard Hamiltonian with a pure Aharonov-Bohm flux ϕ (in units of ϕ_0) without any Zeeman term. The magnetic vector potential modifies the hopping integral by a phase factor and the Hamiltonian for a N-site ring becomes

$$H = t \sum_{\sigma} \sum_{i=1}^{N} (c_{i,\sigma}^{\dagger} c_{i+1,\sigma} e^{i\Theta} + h.c.) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}$$
$$+ \sum_{\sigma} \sum_{i=1,3,\dots}^{N-1} (\epsilon_{A} n_{i,\sigma} + \epsilon_{B} n_{i+1,\sigma})$$
(1)

Here $c_{i\sigma}^{\dagger}(c_{i\sigma})$ is the creation (annihilation) operator and $n_{i\sigma}$ is the number operator for the electron in the Wanniar state $|i\sigma\rangle$. The parameters t and U are respectively the nearest-neighbor hopping integral and the strength of Hubbard correlation, and, ϵ_A and ϵ_B

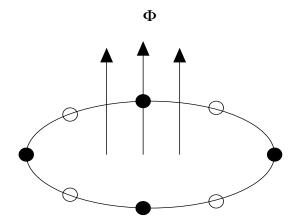


Figure 1: Schematic diagram of a 1D ordered binary alloy ring threaded by magnetic flux ϕ .

are the site potentials for the A and B type atoms. The phase factor is $\Theta = 2\pi\phi/N$. Henceforth, we take t=-1 and use the units c=e=h=1. We always choose N to be even so as to preserve the perfect binary ordering of the two types of atoms in the ring (see Fig. 1).

At zero temperature, persistent current in an isolated ring threaded by magnetic flux ϕ is given by [3]

$$I(\phi) = -\frac{\partial E_0(\phi)}{\partial \phi},\tag{2}$$

where $E_0(\phi)$ is the ground state energy. We calculate $I(\phi)$ exactly by numerical diagonalization of the Hamiltonian.

Let us now study the behavior of persistent currents in the ordered binary alloy rings, and investigate the role of electron-electron interaction on the currents. In a pure ring consisting of either A or B type atoms without electron correlation, the persistent current as a function of ϕ is discontinuous at certain points due to ground state degeneracy, and, the $I-\phi$ curve exhibits a saw-tooth like behavior[3]. In a binary alloy ring with U=0, this discontinuity completely disappears as illustrated in Fig. 2(a) by the solid curve. The reason for this is that the binary alloy configuration may be considered as a perturbation over the perfect ring which lifts the ground state degeneracy, and consequently, makes $I(\phi)$ a continuous

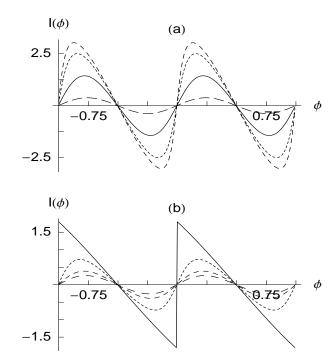


Figure 2: The $I-\phi$ curves of four $(\uparrow,\uparrow,\downarrow,\downarrow)$ electron ordered binary alloy rings. (a) N=4, $N_e=4$. The solid, dotted, small dashed and dashed lines correspond to U=0, 2, 4 and 10 respectively, and (b) N=8, $N_e=4$. The solid, dotted, small dashed and dashed lines are respectively for U=0, 2, 4 and 6.

function of ϕ . As we switch on the electron-electron interaction in a pure ring, persistent current always decreases with the increase of U. However, in the ordered binary alloy rings, depending on the number of electrons N_e , we observe enhancement of the persistent current for low values of U, but eventually it decreases when U becomes very large. Such a situation is depicted in Fig. 2(a) where we display the $I-\phi$ curve for a half-filled ordered binary alloy ring with four electrons (two up and two down spin electrons). Here we see that for U=2 (dotted line) and U=4 (small dashed line), the current amplitudes are significantly larger than the non-interacting case, whereas for U=10 (dashed line) the current am-

plitude is less than that from the U=0 case. This enhancement takes place above quarter-filling, i.e., when $N_e > N/2$, and can be easily understood as follows. As N is even, there are exactly N/2 number of sites with the lower site potential energy. If we do not take into account the electron-electron interaction then above quarter-filling, it is preferred that some of these lower energy sites will be doubly occupied in the ground state. As we switch on the Hubbard correlation, the two electrons that are on the same site repel each other and thus causes enhancement of persistent current. But for large enough U, the electron-hopping is strongly suppressed by interaction, and the current gets reduced. On the other hand, at quarter-filling and also below quarter-filling, no lower energy site will be doubly occupied in the ground state and hence there is no possibility of enhancement of persistent current due to Coulomb repulsion. In these systems we always get suppression of persistent current with the increase of interaction strength U. In Fig. 2(b), we plot the $I-\phi$ curves for a guarter-filled binary-alloy ring with U=0, 2, 4 and 6, and it clearly shows that the persistent currents are always suppressed by interaction.

Let us now describe the behavior of persistent current with system size N in the ordered binary-alloy rings keeping N_e/N constant. For this purpose we calculate current amplitude I_0 at some typical value of magnetic flux $\phi = 0.25$ and in Fig. 3 we plot the I_0 versus N curves. The results for the non-interacting rings are presented in Fig. 3(a), where the solid and dashed lines correspond the rings of size $N = 4N_e$ and $N = 4N_e + 2$ respectively. Since the dimension of the Hamiltonian matrices for the interacting systems increases very sharply with N for higher number of electrons N_e and also the computational operations are so time consuming, we present the variations for the interacting rings with size $N = 2N_e$ only. In Fig. 3(b) the results for the interacting rings are plotted. The solid and dotted lines, representing the results respectively for the rings with U = 0.2and U = 0.6, almost coincide with each other, while, those results for the rings with U = 1.5 and U = 3are respectively represented by the small dashed and dashed lines. These results can predict the variations of current amplitude for the rings with size $N = 4N_e$

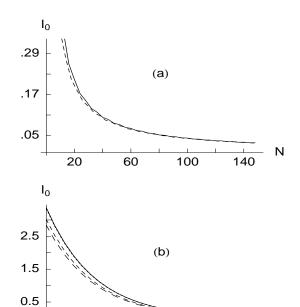


Figure 3: Current amplitude I_0 as a function of system size N in ordered binary-alloy rings. (a) The solid and dashed lines correspond the non-interacting rings of size $N=4N_e$ and $N=4N_e+2$ respectively. (b) The solid, dotted, small dashed and dashed lines correspond the interacting rings of size $N=2N_e$ with $U=0.2,\ 0.6,\ 1.5$ and 3 respectively.

8

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and also $N=4N_e+2$. It is apparent from Fig. 3 that the current amplitude gradually decreases with system size i.e., we get a converging behavior of current amplitude with N and most interestingly we see that in the interacting rings current amplitude converges to zero for any non-zero value of U. These results predict that in a realistic bulk system I_0 goes to zero as soon as the interaction is turned on.

3 Rings with incommensurate site potentials

In this section, we study persistent currents in 1D rings with quasi-periodic site potentials, and investi-

gate the effects of electron-electron interaction on the currents. We describe a N-site ring with incommensurate site potentials by the Hamiltonian

$$H = t \sum_{\sigma} \sum_{i=1}^{N} (c_{i,\sigma}^{\dagger} c_{i+1,\sigma} e^{i\Theta} + h.c.)$$
$$+ \sum_{\sigma} \sum_{i=1}^{N} \epsilon \cos(i\lambda \pi) c_{i,\sigma}^{\dagger} c_{i,\sigma} + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}$$
(3)

where λ is an irrational number, and as a typical example we take it as the golden mean $\left(\frac{1+\sqrt{5}}{2}\right)$. Setting $\lambda=0$ we get back the pure ring with identical site potential ϵ .

To understand the precise role of electron-electron interaction on persistent current in the presence of incommensurate site potentials, let us first consider the simplest possible system which is the case of a ring with two opposite spin electrons. In Fig. 4 we plot the $I - \phi$ curves for a 30-site incommensurate ring with U=0 (solid line), U=1 (dotted line), and U=3 (dashed line). In the absence of any interaction, persistent current is greatly reduced by the incommensurate site potential, and in fact, Fig. 4 shows that the $I - \phi$ curve for the non-interacting case (solid line) almost coincides with the abscissa. This result can be easily understood from the argument that in the presence of aperiodic site potentials, the electronic eigenstates are critical [21, 22] which tends to localize the electrons, and thus reduces the current. But this situation changes quite dramatically as we switch on the electron-electron interaction. Fig. 4 clearly shows that electron correlation considerably enhances persistent current for low values of U. This is because the repulsive Coulomb interaction does not favor double occupancy of the sites in the ground state, and also it opposes confinement of the electrons due to localization. Thus the mobility of the electrons increases as we introduce Hubbard correlation and gives enhancement of persistent current. But this enhancement ceases to occur after certain value of U due to the ring geometry, and persistent current then decreases as we increase U further. We also observe that some strange kink-like structures appear in the $I-\phi$ characteristics around $\phi = \pm 0.5$ for non-zero values of U. Quite sur-

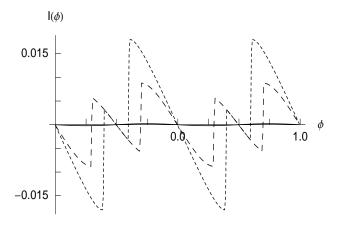


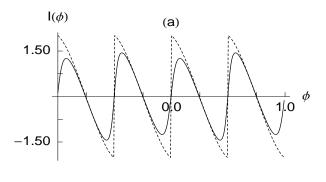
Figure 4: The $I - \phi$ curves for two (\uparrow, \downarrow) electron incommensurate rings with N = 30. The solid, dotted and dashed lines are respectively for U = 0, 1, and 3.

prisingly we notice that the persistent currents inside these kinks are independent of the strength of Hubbard correlation U. Let us now analyze this result. For two opposite spin electrons, total spin S can have the values S=0 and 1. The Hamiltonian of this system for any ϕ can be block diagonalized by proper choice of the basis, and this can be achieved by taking all the basis states in one sub-space with S=0, while those in the other sub-space with S = 1. It is easy to see that in the sub-space spanned by the basis set with S=1, the block Hamiltonian is free from U, and, the corresponding energy eigenvalues and eigenstates are U-independent. In the absence of interaction, these U-independent energy levels are always above the ground level for any ϕ . But for nonzero values of U, one of these U-independent energy levels becomes the ground state energy of the system in certain domains of ϕ . In these regions we have kinks in the $I - \phi$ curves, and it is obvious that the persistent currents inside these kinks are independent of the Hubbard correlation U. We observe that interaction does not alter the ϕ_0 periodicity of persistent current in this two-electron system.

Next we consider incommensurate rings with two up and one down spin electrons as the representative examples of three-electron systems. The $I-\phi$

characteristics for the half-filled (i.e., $N = 3, N_e = 3$) system with U = 4 are shown in Fig. 5(a). In this figure, the dotted line corresponds to a pure ring which exhibits discontinuous jumps at $\phi = 0, \pm 0.5$ due to the crossing of the energy levels. Interestingly, we observe that this pure $(\lambda = 0)$ half-filled three-electron system exhibits a perfect $\phi_0/2$ periodicity, and we will see that this is a characteristic feature of the pure half-filled systems with odd number of electrons. It is evident from the solid curve of Fig. 5(a) that this $\phi_0/2$ periodicity no longer exists as we introduce the incommensurate site potentials, and we have the usual ϕ_0 periodicity. Moreover, in this case $I(\phi)$ becomes a continuous function of ϕ as the perturbation due to disorder lifts the ground state degeneracy at the crossing points of the energy levels. The characteristic features of the persistent currents are quite different in the non-half-filled rings with two up and one down spin electrons, and in Fig. 5(b) we present the results for a 12-site ring with incommensurate site potentials. The solid line is the $I-\phi$ curve for the non-interacting electrons (U=0), while the dotted and dashed lines represent the $I-\phi$ curves for U=4 and U=50 respectively. The role of electronelectron interaction on persistent current in the presence of incommensurate site potentials becomes evident from these curves. For low values of U, the $I-\phi$ curve resembles to that for the non-interacting case, and the persistent currents do not show any discontinuity. But for large enough U, kink-like structures appear in the $I-\phi$ characteristics as illustrated in Fig. 5(b) by the dashed line, e.g., around the point $\phi = 0$. In this case also, the kinks are due to the U-independent eigenstates like the two electron systems, and as explained earlier, the currents inside the kinks are independent of the strength of correlation U. It is observed that the persistent currents always have the ϕ_0 periodicity in the non-half-filled systems. We also notice that for the half-filled systems, persistent currents always decrease as we increase U, while in the non-half-filled rings we obtain significant enhancement of the currents due to interplay between electron correlation and the incommensurate site po-

As a systematic approach, next we investigate the behavior of persistent currents in four-electron sys-



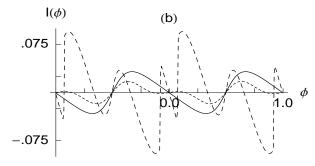


Figure 5: The $I-\phi$ curves for three $(\uparrow,\uparrow,\downarrow)$ electron incommensurate rings. (a) Half-filled (N=3) systems with U=4. The dotted and solid lines corresponds to $\lambda=0$ and $\lambda\neq 0$ respectively. (b) Nonhalf-filled (N=12) systems with $\lambda\neq 0$. The solid, dotted and dashed lines are respectively for U=0,4, and 50.

tems with incommensurate site potentials, and as the representative examples we consider rings with two up and two down spin electrons. The $I-\phi$ curves for the half-filled systems are plotted in the Fig. 6(a). The solid, dotted and dashed lines are for the cases with $U=0,\ U=4$ and U=10 respectively. It is evident from these curves that the current amplitude gradually decreases with the increase of interaction strength U. This indicates that in the half-filled systems, the mobility of the electrons gradually decreases with the increase of U, and we see that for large enough U, the half-filled system goes to an insulating phase. This kind of behavior holds true in

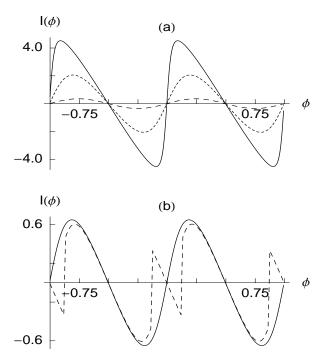


Figure 6: The $I-\phi$ curves for four $(\uparrow,\uparrow,\downarrow,\downarrow)$ incommensurate rings. (a) Half-filled (N=4) systems. The solid, dotted and dashed lines corresponds U=0,4 and 10 respectively. (b) Non-half-filled (N=8) systems. The solid and dashed lines are respectively for U=4 and 16.

any half-filled system because at large enough U, every site will be occupied by a single electron and the hopping of the electrons will not be favored due to strong electron-electron repulsion. In Fig. 6(b), we display the $I-\phi$ curves for the non-half-filled four-electron systems with the aperiodic Harper potential. The solid and dotted lines are the $I-\phi$ curves for a 8-site ring with U=4 and U=10 respectively. This figure depicts that for low U persistent current $I(\phi)$ has no discontinuity, but kinks appear in the $I-\phi$ curve at large U. These kinks arise at sufficiently large U due to additional crossing of the ground state energy levels as we vary ϕ . It may be noted that in the present case kinks are due to the U-dependent

states, and not from the U-independent states as in the previous cases. Both for the half-filled or non-half-filled incommensurate rings with four electrons, we observe that the persistent currents always exhibit ϕ_0 periodicity.

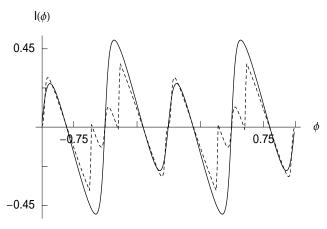
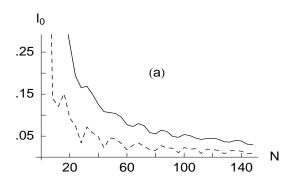


Figure 7: The $I - \phi$ curves for five $(\uparrow, \uparrow, \uparrow, \downarrow, \downarrow)$ electron incommensurate rings. The curves are for the non-half-filled (N = 7) systems. The solid and dotted lines are respectively for U = 18 and 120.

Lastly, we consider five electron aperiodic rings, and calculate persistent currents in rings with three up and two down spin electrons. In the pure halffilled case (i.e., $N = 5, N_e = 5$ and $\lambda = 0$) we get $\phi_0/2$ periodicity in persistent current, and we have already observed such period halving in other pure half-filled systems with odd number of electrons (e.g., $N=3, N_e=3$ and $\lambda=0$). Like the three-electron half-filled incommensurate systems, also in this case the ϕ_0 periodicity of persistent current is restored once we introduced incommensurate site potentials. The $I-\phi$ curves for the non-half-filled five-electron systems with N=7 are shown in Fig. 7. The solid and dotted lines are respectively for the cases with U=18 and U=120. As in the non-half-filled threeelectron system, here also kinks appear in the $I-\phi$ curves above some critical value of U. Another important observation is that for large U (U = 120), the maximum amplitude of the current remains finite. This is quite natural since we are considering the systems with $N>N_e$ where some sites are always empty so that electrons can hop to the empty site, and thus the system always remains in the conducting phase. We also see that in these non-half-filled five-electron rings persistent currents always have the ϕ_0 periodicity.



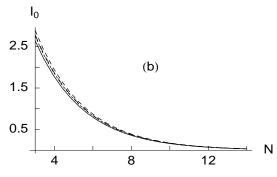


Figure 8: I_0 versus N curves for the systems with incommensurate site potentials. (a) Non-interacting rings, where the solid and dashed lines correspond the rings of size $N=2N_e$ and $N=4N_e$ respectively. (b) The solid, dotted, small dashed and dashed lines correspond the interacting rings of size $N=2N_e$ with $U=0.2,\ 0.6,\ 1.5$ and 6 respectively.

Now we address the behavior of persistent current with system size N keeping N_e/N constant, for the rings with incommensurate site potentials. Like ordered binary-alloy rings here we determine the current amplitude I_0 at some typical value of $\phi = 0.25$ and Fig. 8 displays the I_0 versus N curves. The solid and dashed lines in Fig. 8(a) respectively corre-

spond the results for the non-interacting rings of size $N=2N_e$ and $N=4N_e$. On the other hand the variations of the interacting rings with size $N=2N_e$ are shown in Fig. 8(b). In this figure the solid, dotted, small dashed and dashed lines correspond the results for the rings with $U=0.2,\ 0.6,\ 1.5$ and U=6 respectively. These curves reveal that the current amplitude gradually decreases with system size N and for large value of N it eventually drops to zero value. Thus here we also get a converging nature of current with the size of the systems and we can say that the current amplitude I_0 converges to zero for any non-zero value of U for large N. Thus these results also predict that in a realistic bulk system I_0 vanishes as soon as the interaction is switched on.

4 Conclusions

In conclusion, we have studied exactly the characteristic features of persistent currents in aperiodic and ordered binary alloy rings in the presence of electron-electron interaction. These systems, which are neither pure nor disordered rings, have welldefined structural order, and, our study yields many interesting results due to interplay between electronelectron interaction and disorder in these systems. Our main results are: i) In the absence of interaction, the discontinuity in $I(\phi)$ as a function of ϕ disappears due to disorder. This has been observed both in the ordered binary alloy rings and also in the aperiodic rings. ii) In pure rings with electron correlation, we observe both ϕ_0 and $\phi_0/2$ periodicities in the persistent currents. However, in the incommensurate and ordered binary alloy rings persistent currents always have the ϕ_0 periodicity. iii) In the ordered binary alloy rings, above quarter-filling we get enhancement of persistent current for small values of U, and the current eventually decreases when U becomes large. On the other hand, below quarter-filling and also at quarter-filling, persistent current always decreases with the increase of U. iv) An important finding is the appearance of kink-like structures in the $I-\phi$ curves of the incommensurate rings only when we take into account electron-electron interaction. Quite surprisingly we observe that in some cases the

persistent currents inside the kinks are independent of the strength of the interaction. These kinks give rise to anomalous Aharonov-Bohm oscillations in the persistent current, and recently Keyser et al. [20] experimentally observed similar anomalous Aharonov-Bohm oscillations in the transport measurements on small rings. v) The current amplitude gradually decreases with N both for the non-interacting and interacting rings, keeping N_e/N constant, i.e., we get a converging behavior of current with the size of the rings. Most interestingly, we predict that in the realistic bulk systems I_0 vanishes as soon as the interaction is switched on. Thus the current amplitude vanishes for a ring of macroscopic size.

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